

Modelling supercritical geothermal flows using TOUGH2

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## MODELLING SUPERCRITICAL GEOTHERMAL FLOWS USING TOUGH2

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**SUMMARY** – There is growing interest in the development of deep geothermal resources, and a related need for models of them. At the high pressures and temperatures found in such systems, supercritical conditions can occur, which most numerical geothermal simulators are not presently capable of modelling. This paper describes a new modified version of the TOUGH2 simulator, capable of modelling supercritical conditions. The modifications are based around the updated IAPWS-97 thermodynamic formulation, and the use of density and temperature as primary thermodynamic variables under supercritical conditions. Results from a suite of test problems are in agreement with the work of other authors. This gives confidence that the simulator can be used for modelling deep geothermal reservoirs.

### 1. INTRODUCTION

As interest grows in the development of largely-untapped deep geothermal resources (at depths of over 3 km), there is a corresponding need for models of deep geothermal systems. At the high pressures and temperatures encountered at these depths, supercritical conditions may occur, in which the distinction between liquid and vapour phases ceases to exist. However, most popular numerical geothermal reservoir simulators (e.g. TOUGH2 (Pruess, 1991), TETRAD (Vinsome, 1990)) limit themselves to sub-critical conditions only.

This paper describes a version of the TOUGH2 simulator which has been modified to model supercritical conditions, extending its applicability to modelling deep geothermal reservoirs, using a new approach and an updated thermodynamic formulation.

### 2. METHODS

#### 2.1 Previous supercritical simulators

The finite-difference HYDROTHERM package (Hayba and Ingebritsen, 1994) was the first widely-available geothermal simulator with two-phase and supercritical modelling capabilities. Pritchett (1994) also described a supercritical extension (HOTH2O) to the finite-difference STAR geothermal simulator. Over the years there has been steady interest in adding supercritical capabilities to the finite-volume MULKOM simulator (Pruess, 1983) and its successor TOUGH2 (Pruess, 1991), in order to take advantage of their ability to deal with irregular computational grids in one, two or three dimensions.

Cox and Pruess (1990) produced a modified version of MULKOM, using interpolated look-up tables based on the supercritical equation of state of Haar et al. (1984). They had mixed success in modelling a near-critical laboratory experiment

carried out by Dunn and Hardee (1981). Kissling (2004) suggested that this may have been partly due to inaccuracies in the look-up table method used.

Brikowski (2001) developed a supercritical equation of state module for TOUGH2 using a set of Taylor-series approximations for supercritical fluid properties published by Johnson and Norton (1991). This produced convincing results for sub- and supercritical 'five-spot' injection-production tests, but suffered from convergence problems near the critical point, and required large amounts of computation time.

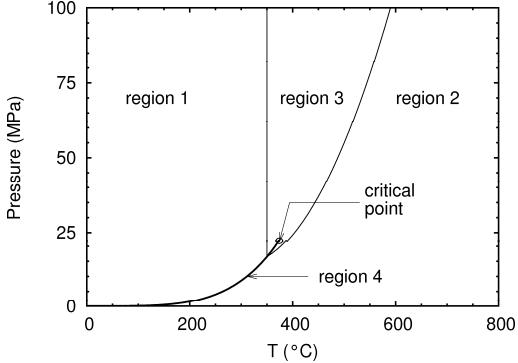
Another supercritical version of TOUGH2 was developed by Kissling (2004). It retained the original thermodynamic formulation used in TOUGH2, the International Formulation Committee 1967 (IFC-67) equations (Arnold, 1970). The IFC-67 formulation included equations for supercritical fluid up to 800 °C and 100 MPa, but these were omitted from standard TOUGH2. Kissling's version included them, and supplemented them with the formulation of Haar et al. (1984) to extend the range of the simulator up to 2000 °C and 200 MPa. The resulting simulator was used to model the Taupo Volcanic Zone geothermal system to a depth of 8 km (Kissling and Weir, 2005).

#### 2.2 IAPWS-97 formulation

In 1997 the IFC-67 thermodynamic formulation was superseded by the IAPWS-97 formulation (Wagner et al., 1997), which was designed to have the same operating range as IFC-67, but greater accuracy and computational efficiency. One of the design requirements was that IAPWS-97 should be at least three times faster than IFC-67 (except close to the critical point).

The IAPWS-97 formulation is also somewhat simpler than IFC-67, in that it divides its operating range into four 'regions' (see Figure 1), where IFC-67 used five (including an additional 'near-

critical liquid' region). The four regions correspond nominally to 1: liquid, 2: steam, 3: supercritical and 4: two-phase. (In fact IAPWS-97 includes a small additional region between 800°C and 2000 °C, and pressure from 0 to 10 MPa, intended for calculations involving gas turbines, but that is not considered here.)



**Figure 1: Main operating range of the IAPWS-97 thermodynamic formulation**

Because of its greater simplicity, and increased accuracy and efficiency, IAPWS-97 was chosen as the thermodynamic formulation for the supercritical version of TOUGH2 developed in the present work.

### 2.3 Primary variables

In the liquid and steam regions, standard TOUGH2 uses pressure and temperature as its primary thermodynamic variables (pressure and saturation in the two-phase region). All other fluid properties are calculated in terms of these variables. For the supercritical region, however, to avoid numerical difficulties near the critical point, both the IFC-67 and IAPWS-97 formulations are given in terms of density and temperature. If pressure and temperature are retained as the primary variables for the supercritical region, this means that fluid density cannot be explicitly calculated from the primary variables. An iterative procedure is needed, which was the approach taken by Kissling (2004). This entails added computational cost, although it is not necessarily significant. For many problems (particularly large ones) the time spent in the thermodynamic routines is small relative to the time spent solving the resulting large systems of linear equations at each iteration.

The approach taken in the present work is to switch to density and temperature as primary variables in the supercritical region, avoiding the need for iteration. The procedure used to switch variables when entering or leaving the supercritical region is similar to that used in standard TOUGH2 when entering or leaving the two-phase region. The calculation is stopped on the boundary between the two regions, the variables are switched, and the calculation is restarted in the new region.

Standard TOUGH2 is written in such a way that the first primary variable is always assumed to be pressure. Before density could be used as the first primary variable in the supercritical region, this constraint had to be relaxed. The required modifications to the TOUGH2 code were carried out along lines similar to those described by Talman et al. (2004) in their application of TOUGH2 to modelling geological storage of CO<sub>2</sub>.

## 3. RESULTS

The new simulator was tested on a range of example problems reported in the literature. Results for three of these problems are shown here.

### 3.1 Near-critical horizontal column

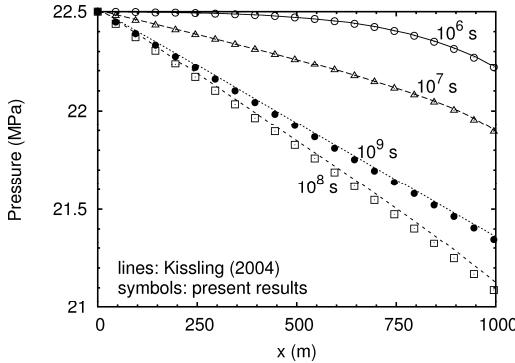
As a first test problem, Kissling (2004) simulated the flow of near-critical fluid in a one-dimensional horizontal column. The column is 1 km long, made up of 100 cube-shaped blocks with side length 10 m. Fluid is extracted from one end ( $x = 1000$  m) at a rate of 0.005 kg/s, with conditions at the other end ( $x = 0$ ) held constant. The rock has permeability  $5 \times 10^{-15}$  m<sup>2</sup>, porosity 0.01, grain density 2650 kg/m<sup>3</sup>, heat capacity 1000 J/kg.K and thermal conductivity 3 W/m.K.

The column is initially at temperature 374 °C and pressure 22.5 MPa. According to the IFC-67 formulation, which Kissling's simulator used, this is just below the temperature at the critical point (374.15 °C, 22.12 MPa). However, the IAPWS-97 formulation locates the critical point at a slightly lower temperature and pressure (373.95 °C, 22.06 MPa). This means that, for the present results, the initial conditions are in fact in the supercritical region.

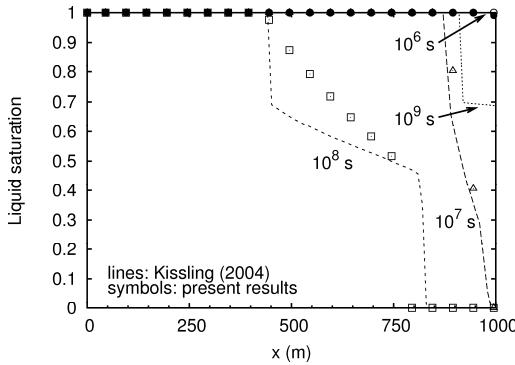
Figure 2 - Figure 5 compare the present solution of this problem with that of Kissling (2004), at times  $10^6$ ,  $10^7$ ,  $10^8$  and  $10^9$  seconds. (Note that the solution times reported in Kissling (2004) were incorrect, being too large by a factor of  $10^6$  due to an error in grid block volumes (Kissling, pers. comm.).)

It can be seen that the pressures and flows of the two solutions agree closely. Temperatures are also in agreement except for some slight differences around the steam/ two-phase boundary at  $10^8$  s.

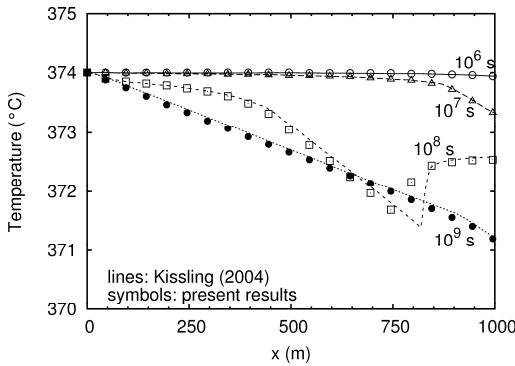
There are noticeable differences in liquid saturations, however, with the present results showing a less sharp boundary between the liquid and two-phase regions at  $10^8$  s. Also, the small steam zone near the production block in Kissling's solution at  $10^9$  s has essentially disappeared in the present results.



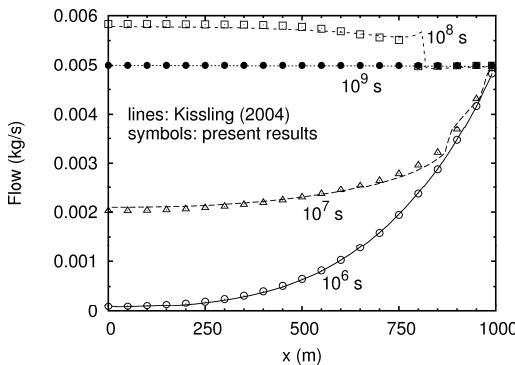
**Figure 2: Horizontal column problem - modelled pressures along column**



**Figure 3: Horizontal column problem - modelled saturations along column**



**Figure 4: Horizontal column problem - modelled temperatures along column**



**Figure 5: Horizontal column problem - modelled flows along column**

These differences are probably due to the fact that the two solutions used different thermodynamic formulations, which locate the critical point at different positions. The problem takes place very near the critical point, where most thermodynamic properties are sensitive to changes in temperature and pressure.

### 3.2 Yano and Ishido problem

Yano and Ishido (1998) modelled the flow from a production well at near-critical conditions, using the HOTH2O extension of the STAR simulator (Pritchett, 1994). They used a radial grid with 40 blocks, 100 m thick, each 1.3 times wider than its inner neighbour, with total radius approximately 12 km. The innermost block (radius 0.1 m) represents the well, with porosity 0.99 and permeability  $10^{-10}$  m<sup>2</sup>. The porosity is 0.05 elsewhere. The permeability outside the well is  $10^{-12}$  m<sup>2</sup> inside a skin zone of radius 0.9 m, and  $10^{-14}$  m<sup>2</sup> outside the skin zone. The rock has grain density 2700 kg/m<sup>3</sup>, heat capacity 1000 J/kg.K and thermal conductivity 2.5 W/m.K. Fluid is extracted at 15.7 kg/s.

Figure 6 shows the modelled pressure for three different initial temperature distributions (all with initial pressure 30 MPa). Cases A and C have homogeneous initial temperatures of 300 °C and 400 °C respectively. Case B has initial temperature 300 °C up to 82 m radius, and 400 °C outside that. The figure shows that the present results are in good agreement with those of Yano and Ishido (1998). The results of Kissling (2004) generally show a slightly larger drawdown.

Figure 7 shows pressure results for seven different homogeneous initial temperatures (each with initial pressure 30 MPa). Again the present results agree closely with those of Yano and Ishido (1998), with only some minor discrepancies in the early time results for 500 °C. The results display the expected rise in pressures as the initial temperature is increased up to 400 °C, and the subsequent drop as the temperature is raised above that (due to the increase in kinematic viscosity of supercritical fluid above 400 °C).

Figure 8 shows drawdown results for four different initial pressures, each with homogeneous initial temperature 450 °C. The present results show slightly larger drawdown at early times (less than 1 hr) but are otherwise in good agreement with those of Yano and Ishido (1998).

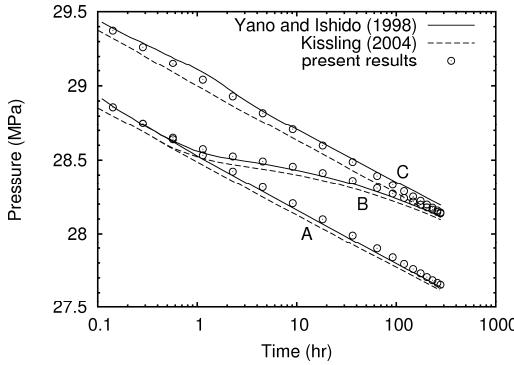


Figure 6: Yano and Ishido (1998) problem-modelled pressure for three initial temperature distributions (A, B, C)

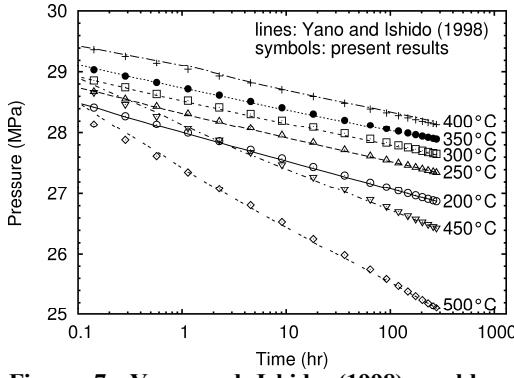


Figure 7: Yano and Ishido (1998) problem-modelled pressure for different homogeneous initial temperatures

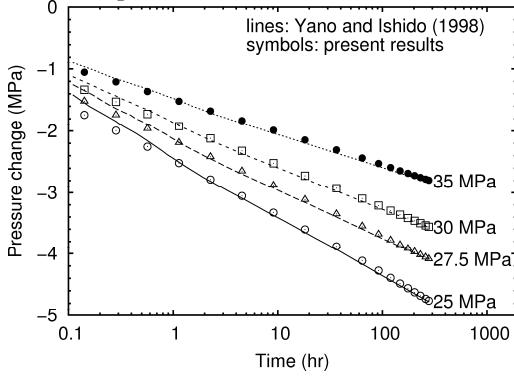


Figure 8: Yano and Ishido (1998) problem-modelled drawdown for different initial pressures

### 3.3 Supercritical five-spot problem

Brikowski (2001) modelled a supercritical version of the 'geothermal five-spot' problem described by Pruess (1991). This problem simulates flow in a large field of injection and production wells arranged in a 'five spot' grid pattern (see Figure 9). Because of the symmetry, this can be modelled using a triangular grid representing one-eighth of the basic pattern (one injection and one production well).

The reservoir is modelled as a porous medium with permeability  $6 \times 10^{-15} \text{ m}^2$  and porosity 0.01. The supercritical version of the problem solved by

Brikowski (2001) uses an elevated initial temperature (400 °C) and pressure (22.06 MPa). Fluid is injected at 0.9 kg/s and produced at the same rate. The injected fluid has enthalpy 500 kJ/kg (i.e. temperature approximately 123 °C).

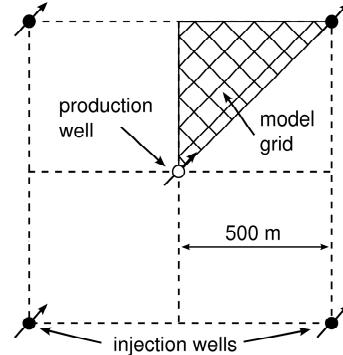


Figure 9: Five spot injection/ production problem

Figure 10 shows a pressure vs. temperature plot of the results. The solid lines represent the results of Brikowski (2001) for the injection well, the production well and a point midway between them ('DA 1'), with the circular symbols representing the corresponding present results.

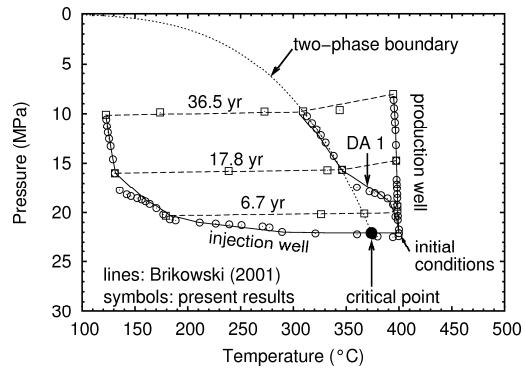


Figure 10: Supercritical five-spot problem-pressure-temperature diagram of modelled results

All three points start at the initial conditions at the lower right and migrate to lower pressures and temperatures, with the injection well passing through the critical point. The midpoint 'DA 1' becomes two-phase, and the production well drops pressure while its temperature remains almost constant. Brikowski's results at three representative times (6.7, 17.8 and 36.5 yr) are joined by dashed lines, with square symbols representing the corresponding present results at selected points between the injection and production wells.

Besides some slight differences at the injection well and the midpoint 'DA 1' between the times 6.7 yr and 17.8 yr, the present results are in very good agreement with those of Brikowski (2001).

Brikowski (2001) also estimated the computational efficiency of his code relative to

standard TOUGH2, by running both simulators on the original sub-critical version of the geothermal five-spot problem, and comparing the elapsed CPU times. Brikowski's code required approximately 20 times more CPU time than standard TOUGH2 for this problem. A similar experiment carried out using the present simulator indicates that it requires only about 83% of the CPU time taken by standard TOUGH2 for this problem (and gives an essentially identical solution). However, this figure will vary depending on the details of the problem solved.

#### 4. CONCLUSIONS

A new supercritical version of the TOUGH2 simulator has been developed using the updated IAPWS-97 thermodynamic formulation. Use of this formulation gives improved accuracy, higher computational efficiency and a simpler representation of the supercritical region. The implementation uses density and temperature as primary thermodynamic variables in the supercritical region, avoiding the iteration needed when pressure and temperature are used.

Results from the new simulator for a range of supercritical test problems are consistent with those published by previous authors. This gives confidence that the simulator can be used for modelling deep geothermal reservoirs. The simulator also runs slightly faster than standard TOUGH2, in contrast to some previous simulators which have been significantly slower than standard TOUGH2.

#### 5. ACKNOWLEDGEMENTS

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